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A method of computational magnetohydrodynamics defining stable Scyllac equilibria

(plasma/high beta stellarator/minimum energy/finite element method/computer code)

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ABSTRACT A computer code has been developed for the numerical calculation of sharp boundary equilibria of a toroidal plasma with diffuse pressure profile. This generalizes earlier work that was done separately on the sharp boundary and diffuse models, and it allows for large amplitude distortions of the plasma in three-dimensional space. By running the code, equilibria that are stable to the so-called $m = 1$, $k = 0$ mode have been found for Scyllac, which is a high beta toroidal confinement device of very large aspect ratio.

In two earlier papers (1, 2) we described a method of steepest descent for the computation of plasma equilibria satisfying the partial differential equations of magnetostatics in three independent variables. The method was based on the standard variational principle of magnetohydrodynamics and yielded primarily stable equilibria. In this paper we synthesize the previous work in order to obtain a more comprehensive computer code that can handle simultaneously a diffuse pressure profile within the plasma and a sharp free boundary separating the plasma from an outer vacuum region. Stability is analyzed by examining global minimum properties of the potential energy. The new code also enables us to study certain unstable equilibria and to discuss growth rates of the associated unstable modes.

So far, no way has been found to improve the performance of confinement systems of the Tokamak class through modifications of the geometry that are not axially symmetric. However, Scyllac equilibria have helical windings that are genuinely three-dimensional and therefore provide an ideal application for our computer code. We have found that the effect of pressureless plasma coupled with large amplitude deformations of the outer coil can be used to stabilize the $m = 1$, $k = 0$ mode, which is a toroidal shift leading to most of the trouble with Scyllac. The code shows that a large so-called $l = 1$ winding combined with a small $l = 2$ winding results in stability when the cross sections of the torus forming the perfectly conducting outer wall have a cloverleaf shape. The required specifications lie within the range of experimental configurations now in operation at the Los Alamos Scientific Laboratory. Modes with higher wave number $m \geq 2$, whose failure to appear in practice is partly due to the effect of finite Larmor radius, are stabilized in runs of the code by the comparable effect of a finite mesh size.

The variational method

Our basic plan is to calculate toroidal equilibria of a plasma by minimizing the potential energy

$$E = \iiint \left[\frac{B^2}{2} + \frac{p}{\gamma - 1} \right] dV$$

in three-dimensional space, subject to appropriate constraints. In the plasma the magnetic field B is represented as the cross product

$$B = \nabla\chi \times \nabla\psi$$

of two flux functions, χ and ψ. The first of these is supposed to be a function $\chi = \chi(s)$ of a single-valued parameter s defining a nested family of toroidal flux surfaces s = const. The pressure p is related to the density ρ by an equation of state, $p = \rho^\gamma$, and the mass between any pair of flux surfaces s = const. is conserved. A sharp interface C can occur between the plasma and an outer vacuum region bounded by a perfectly conducting wall S. The vacuum field is represented as the gradient

$$B = \nabla\phi$$

of a scalar potential ϕ with fixed fluxes. The normal component of B vanishes at all boundaries.

In equilibrium the energy E becomes stationary with respect to admissible perturbations of the magnetic field B, the fluid pressure p, and the free boundary surface C. In the plasma the partial differential equations characterizing equilibrium are

$$\nabla \cdot B = 0, \qquad J \times B = \nabla p$$

in which $J = \nabla \times B$ is the current. In the vacuum these equations become

$$\nabla \cdot B = 0, \qquad \nabla \times B = 0$$

so the function ϕ must be harmonic. The free boundary condition making E stationary with respect to variations of the sharp interface C asserts that the combined fluid and magnetic pressure

$$P = p + B^2/2$$

is continuous across C. Both p and the tangential components of B will in general have jumps there.

The relationship $B \cdot \nabla p = 0$ shows that the magnetic lines are real characteristics of the magnetostatic equations inside the plasma. This causes a difficulty with the variational method that we overcome by imposing the ergodic constraint that p be a function of the flux parameter s alone. Justification of such a step and explanations of other details of the method, such as the construction of ϕ, can be found in previous publications (1, 2). Here we confine our attention to matters essential to an understanding of how the diffuse profile and sharp boundary models have been combined.

Consider a system of modified cylindrical coordinates r, θ, and z defined in terms of rectangular coordinates x, y, and z by the formulas

$$x = (R + r)\cos\theta, \qquad y = (R + r)\sin\theta$$

in which R is a positive number that will measure the major radius of a torus. Put $\theta = 2\pi v$, and assume that the flux parameter s ranges over the interval $0 \leq s \leq 1$, with the minimum value, $s = 0$, corresponding to a magnetic axis which we represent by means of two equations

$$r = r_0(v), \qquad z = z_0(v).$$

Let u be a variable on the interval $0 \leq u \leq 1$ and let

$$r = r_1(u,v), \quad z = z_1(u,v)$$

be a parametric representation of the outer toroidal wall S, where r_1 and z_1 are periodic functions of u and v with unit periods. The flux surfaces s = const. inside the plasma are nested tori whose parametric equations we now write in the form

$$r = r_0(v) + f(u,v,s)g(u,v)[r_1(u,v) - r_0(v)],$$
$$z = z_0(v) + f(u,v,s)g(u,v)[z_1(u,v) - z_0(v)]$$

in which f and g are radial functions that are periodic in u and v and assume values in the range $0 \leq f \leq 1, 0 < g < 1$. In particular, we set $f(u,v,1) = 1$ so that g defines the free surface $s = 1$ separating the plasma from the vacuum. Finally, we introduce coordinates u, v, and s in the vacuum region by means of the formulas

$$r = r_0 + [s - 1 + (2 - s)g][r_1 - r_0],$$
$$z = z_0 + [s - 1 + (2 - s)g][z_1 - z_0]$$

with s ranging over the interval $1 \leq s \leq 2$, where it is no longer related to flux.

The plasma and the vacuum are mapped onto a pair of adjacent cubes in the space with coordinates u, v, and s. For $0 \leq s \leq 1$ the first flux function, χ, depends on s alone, and we take it to have the form

$$\chi = s(1 + \alpha s)$$

with the coefficient α chosen so that the level surfaces s = const. become evenly spaced near the magnetic axis. The second flux function, ψ, is supposed to have the representation

$$\psi = -u + \mu(s)v + \Psi$$

in which $\Psi = \Psi(u,v,s)$ is an unknown function periodic in the variables u and v and defined for $0 \leq s \leq 1$. The factor $\mu = \mu(s)$ is an invariant, called the rotational transform, which is fixed by the flux constraints of the problem. The scalar potential, ϕ, defined for $1 \leq s \leq 2$, has two periods in the variables u and v that are determined so the dual pair of fluxes of the magnetic field B assume prescribed values.

After these transformations have been made, the potential energy becomes a known functional

$$E = E(\phi,\psi,f,g,r_0,z_0)$$

of the three functions ϕ, ψ, and f of three variables, of the single function g of two variables, and of the two functions r_0 and z_0 of a single variable. The contribution to E from the vacuum region has been discussed in some detail in ref. 1, and the contribution to E from the plasma has been described carefully in ref. 2.

Euler equations for ϕ, ψ, f, g, r_0, and z_0 can be found by applying the standard procedure of the calculus of variations to the functional E. Let us write these equations symbolically in the form

$$L_1[\phi] = L_2[\psi] = L_3[f] = 0,$$
$$K(g,g_u,g_v) = M_1[r_0] = M_2[z_0] = 0.$$

We see that L_1 is simply the Laplace operator with respect to the curvilinear coordinates u, v, and s. The pair of second-order partial differential equations for ψ and f defined by the operators L_2 and L_3 are of nonstandard type. The function K depends on the components of the magnetic field at the sharp boundary C, since it is equal to the jump there in the fluid plus magnetic pressure P. However, it is perhaps better to interpret the statement $K = 0$ as a partial differential equation for g of the first order and the second degree. The relationships M_1 and M_2 for the magnetic axis involve averaging processes and are therefore more tractable. It can be shown by example that the full system of magnetostatic equations we have written has weak solutions even in cases in which regularity does not prevail.

Accelerated paths of steepest descent

We propose to calculate magnetohydrodynamic equilibria by considering paths of steepest descent associated with the potential energy E (1, 2). To define the paths of steepest descent we introduce an artificial time parameter t and write partial differential equations for the six unknowns ϕ, ψ, f, g, r_0, and z_0 as functions of the four independent variables u, v, s, and t. The equations are found by adding partial derivatives with respect to the artificial time t to the Euler equations so as to obtain a system of the hyperbolic type. In the case of the equation for the free surface $\bar{C}$, this requires adding a partial derivative $\partial g/\partial t$ of the first order. For the magnetostatic equations, which are of nonstandard type, we must add first- and second-order derivatives of ψ and f that are suggested by the conjugate gradient method. For the potential function ϕ we add mixed partial derivatives with respect to space and time that are characteristic of the method of successive overrelaxation. The entire system can be expressed in the concise form

$$aU_{tt} + bU_{ut} + cU_{vt} + dU_{st} + eU_t = L[U]$$

in which U is the six-dimensional vector of unknowns, L is the differential operator specified by the Euler equations, and a, b, c, d, and e are matrices of parameters controlling the convergence of the solution. To compute physically stable equilibria, the parameters are to be chosen so that E approaches a minimum value and U approaches a steady state as t becomes infinite.

Because it is the fluxes and not the currents of the vacuum magnetic field B that are held fixed, the energy E becomes a maximum as a functional of ϕ rather than a minimum at equilibrium. To use the minimum property of E as a test for stability it therefore becomes necessary in principle to solve the Laplace equation for ϕ exactly for each value of the artificial time. In practice it suffices instead to use appropriate acceleration factors in the choice of the coefficient matrices a, b, c, d, and e. Another alternative, which we have not yet explored in detail, would be to solve the Laplace equation by applying fast Fourier transform with respect to the periodic variables u and v in order to invert the dominant terms.

The role of the coefficients a, b, c, and d in the system of partial differential equations for U is to bring them into the hyperbolic type and provide them with appropriate characteristics. The second-order terms result in an accelerated method of steepest descent for E whose rate of convergence is governed by the first-order coefficient e. Let us suppose that, for large artificial time t, the energy E has an expansion

$$E = \Sigma A_n \exp(2\lambda_n t)$$

in exponential functions. Values of $|E_{tt}/E_t|$ averaged over a number of time cycles are a good measure of the dominant rate 2λ of growth or decay of E. Expansion of U in a similar series of exponentials and substitution of the series into a system of linearized differential equations gives a quadratic equation for the rate of growth or decay λ of U in terms of e that has the form

$$a\lambda^2 + e\lambda = \omega^2$$

in a scalar case with $b = c = d = 0$. Manipulation of this relationship shows that, for fixed a, b, c, and d, the optimal choice for e providing maximal acceleration of the convergence in t

is a quantity proportional to the dominant growth rate λ. When such a law of proportionality between e and $|E_{tt}/E_t|$ is imposed, which means of course that e varies with t, not only is the best rate of convergence achieved but also an estimate is obtained of the growth rate ω of the least favorable mode for an equilibrium that is unstable. To ascribe a physical meaning to this growth rate in practice, comparison must be made with some example in which an Alven transit time is known from other considerations.

The procedure we have described for acceleration by means of a variable convergence factor e enhances significantly the method of steepest descent, which is prohibitively slow in its standard formulation. The procedure is also applicable to the problem of estimating the relaxation factor for the method of successive overrelaxation in a more general context, provided that a functional like E is available to assess the growth rate of the dominant mode in the error, which tends to switch around at different stages of the iteration. In this way, rates of convergence can be improved by as much as a factor of 10 in practice.

An exception to what has been said has to be made for the partial differential equation of the free surface because it is only of the first order. However, no acceleration is called for in that case, so the coefficients of the time derivatives can be assigned in a more obvious way. It then turns out that the previous assertions about growth rates remain valid even with a free surface included in the model. For the free surface model, the convergence of the solution is markedly improved in a coordinate system, such as ours, tied to the motion of the magnetic axis.

Discretization

In order to implement our scheme for the computation of magnetohydrodynamic equilibria numerically, we apply the finite element method to the variational principle for the potential energy E. This is accomplished by first writing down a second order accurate discrete approximation of E, which can be done several different ways using a rectangular mesh. To arrive at finite difference equations for equilibrium, we set equal to zero the derivatives of the approximation of E with respect to the nodal values of the unknowns. A discrete version of the problem is thus obtained which is in conservation form and therefore can be solved even when only weak solutions of the continuous version are presumed to exist. It is especially important to use a conservation form of the magnetostatic equations inside the plasma (2). Conservation form is also required of the Laplace equation for the potential ϕ of the vacuum magnetic field because of the familiar compatibility condition on the solution of the Neumann problem. However, more latitude is permissible in the numerical treatment of the free boundary condition.

An iterative scheme to solve the finite difference equations for equilibrium is obtained by adding in difference approximations of the artificial time derivatives used to define paths of steepest descent. For a given choice of the mesh sizes in u, v, s, and t, the coefficients a, b, c, and d must be selected to meet the Courant-Friedrichs-Lewy criterion for numerical stability and convergence. Then, an estimate of E_{tt}/E_t can be used to determine the coefficient e so as to give optimal convergence of the iterations. In physically unstable cases the method diverges, but it yields an estimate of the growth rate of the most unfavorable mode.

Again an exception must be made of the first-order equation for the free surface, which we take to have the form

$$g_t = K(g, g_u, g_v).$$

Since no second-order derivatives with respect to artificial time appear, it is now the relevant element of e that has to be selected to meet the Courant-Friedrichs-Lewy criterion. We have normalized it to be unity. Moreover, differencing must be performed in a fashion appropriate for equations of the first order. We have used a version of the Lax-Wendroff scheme involving averages of the nodal values of K that lead to stability attributable to weights dependent on $\partial K/\partial g_u$ and $\partial K/\partial g_v$. This introduces relatively little artificial viscosity, but a certain amount seems unavoidable for any successful computation of free surfaces in space of dimension higher than two (1). It is significant that, for both the first-order and the second-order partial differential equations of the full artificially time-dependent system for U, the Courant-Friedrichs-Lewy stability criterion simply imposes uniform bounds on the ratios of the mesh size in artificial time to that in the space variables.

Mathematical instabilities of the numerical method we have described are easily distinguished from physical instabilities of the equilibrium being computed because the former tend to make E oscillate or increase whereas the latter always make E decrease indefinitely. A finer analysis of the solution can be performed by plotting Fourier coefficients of important geometric and physical quantities as functions of the artificial time on a logarithmic scale. However, to obtain good resolution, the mesh sizes and convergence factors occurring in the method must be adjusted sensibly.

The effect of finite mesh size is to introduce truncation errors that we can liken to artificial elasticity. This is comparable to the effect of finite Larmor radius in plasma physics and tends to make equilibria seem more stable in the calculations than they actually are for the continuous magnetohydrodynamic model. Theoretically the truncation error can always be assessed by refining the mesh, but limitations on computer capacity for large-scale, time-dependent calculations in three dimensions restrict what can be achieved in practice.

We have written a Fortran code for the CDC 6600 computer that implements the ideas described above for the numerical calculation of sharp-boundary diffuse-profile equilibria of a toroidal plasma. The code has been validated through extensive comparisons with exact solutions of the magnetostatic equations and with normal mode analyses of linear stability. A typical run of 1000 artificial time cycles on a mesh of 6000 grid points takes about an hour of machine time. The code has been distributed to the Los Alamos Scientific Laboratory and can be obtained from the Argonne Code Center of the Argonne National Laboratory.

Stable high β equilibria

The computational method we have described is useful for the determination of high β equilibria, where β refers to a standard value of the dimensionless parameter $\beta = 2p/B^2$. For low aspect ratio toroidal devices of the Tokamak class we have found stable sharp boundary equilibria with β as high as 0.25. This is achieved with axially symmetric geometry by denting in the container wall along its outer perimeter. However, the plasma fills half the volume of the container and therefore comes perhaps unrealistically close to the outer wall in equilibrium. Also, there are difficulties in heating such a plasma.

More fruitful applications of the method have been made to large aspect ratio, high β stellarators like the Scyllac developed at Los Alamos (3). The equilibrium and stability code can be used to model one period of Scyllac consisting of a slightly bent and twisted section of a cylinder. In the vacuum we put equal to zero the flux dual to the current

$$I = \oint d\phi$$

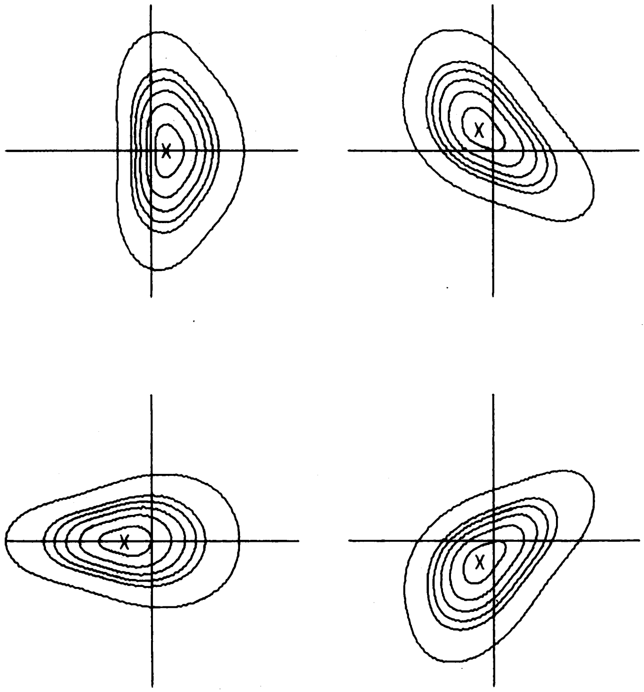

FIG. 1. Sample cross sections of coil stabilizing pressureless plasma model of Scyllac.

obtained by integrating over a cycle that is as short as possible. Correspondingly, in the plasma we make the rotational transform μ vanish identically. Letting R become the aspect ratio, we write the equations of the outer wall S in the form

$$r_1(u,v) = (1 - \Delta_0 \cos 2\pi v)[\cos 2\pi u - \Delta_2 \cos 2\pi(u - v)] + \Delta_1 \cos 2\pi v + \Delta_3(\cos 2\pi u) \cos 6\pi(u - v).$$

$$z_1(u,v) = (1 - \Delta_0 \cos 2\pi v)[\sin 2\pi u + \Delta_2 \sin 2\pi(u - v)] + \Delta_1 \sin 2\pi v + \Delta_3(\sin 2\pi u) \cos 6\pi(u - v)$$

in which the wavelength of the Δ_3 term is somewhat unconventional. Here $2\pi v/\theta$ represents the number of periods of the device and is no longer unity. The shape factors Δ_1 and Δ_3 describe an l , 1 coil that has helical symmetry, whereas the coefficients Δ_0 and Δ_2 introduce additional $l = 0$ and $l = 2$ fields.

The computer code shows that stable equilibria for Scyllac exist when the outer region is filled mostly with pressureless plasma and there is only a relatively thin vacuum shell. For example, a stable configuration near one being tested at Los Alamos has been found with 24 periods, $R = 37$, $\beta = 0.6$, $\Delta_0 = 0$, $\Delta_1 = 0.23$, $\Delta_2 = 0.3$, and $\Delta_3 = 0.1$. The geometry of this case is illustrated in Fig. 1, where the next to the last flux surface represents the free boundary. Characteristic of the stable equilibria is the fact that the cross sections of the helical $l = 1$ coil are not perfectly circular. The results suggest that perhaps the least stable straight helical equilibria for the pressureless plasma model are those with circular cross sections.

The most remarkable feature of our equilibria is their stability to the $m = 1$, $k = 0$ mode, which is an infinitesimal translation in the r,z plane. This mode is sensitive to the number of mesh points in the direction of v; too few can make it appear more stable than it really is. Similarly, the effect of a relatively large mesh size in u is to stabilize the $m = 2$ mode, which is also subject to damping by the diffuse pressure profile. This effect has been verified by investigating a case in which $\mu \equiv 1/2$. Typical runs on which our stability analysis is based have 32 mesh intervals in the poloidal and toroidal coordinates u and v but 16 in the radial flux coordinate s.

Unstable Scyllac equilibria can also be studied by means of the code. This is done by initializing the average coordinates of the magnetic axis at different positions along the r axis. The

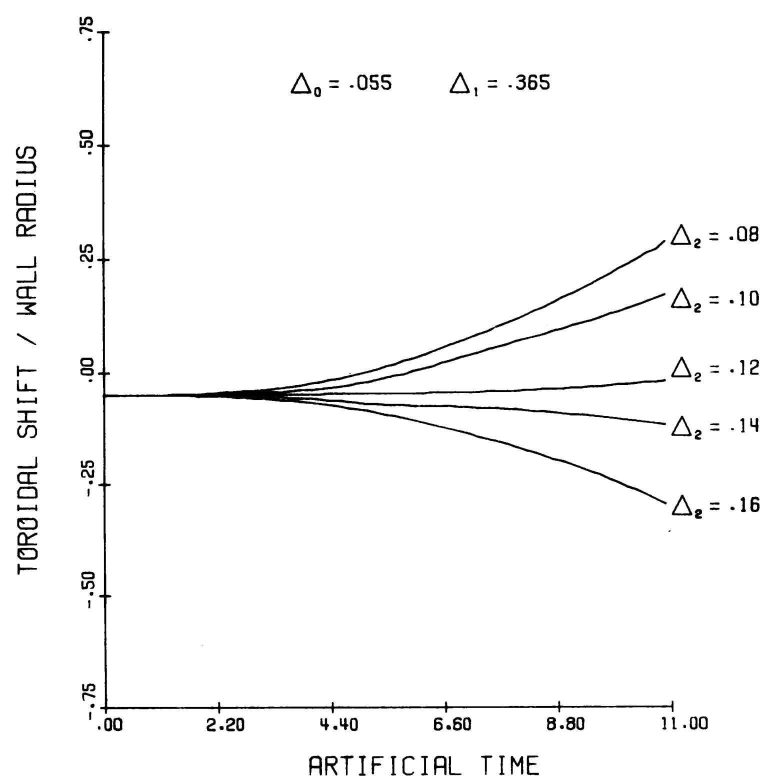

FIG. 2. Streak plot of plasma displacement for computer model of Garching experiment.

plasma moves inward with advancing artificial time when the magnetic axis is located initially far enough in toward the major toroidal axis, whereas it moves outward when the initial position lies further out. At some intermediate position the magnetic axis hovers longer before moving in either direction. This behavior is interpreted to indicate the presence of an unstable equilibrium near the intermediate position, a conclusion that is borne out by closer examination of the forces that occur. We have found the toroidal restoring force required for equilibrium to be somewhat bigger than that predicted by linearized sharp boundary theory when the helical excursion Δ_1 is large (4–6). Because these results are sensitive to truncation error, longer runs on a mesh of 16,000 points have been necessary to establish them convincingly. There is also sensitivity to the initial shape of the magnetic axis; too little helical excursion makes it move in, whereas too much makes it move out.

We have compared our computer simulation of unstable equilibria with experimental data from the Max Planck Institute for Plasma Physics in Garching (7). Quite good agreement was obtained between the magnitude of the $l = 2$ field required for equilibrium in the experiment and the corresponding value of the shape factor Δ_2 needed for equilibrium according to the theory. Results of our computational analysis of the Garching high β stellarator are shown in Fig. 2.

We have estimated growth rates of the $m = 1$, $k = 0$ mode for unstable equilibria. These can be compared with the times of duration of the corresponding experiments, which run between 5 and 20 μsec. The hope would be that, if a stable equilibrium surrounded by pressureless plasma were tested with a correct analysis of the necessary restoring force, then the experiment might last more than 100 μsec.

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